Comparison with other packages

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library(phylosem)

phylosem is an R package for fitting phylogenetic structural equation models (PSEMs). The package generalizes features in existing R packages:

- sem for structural equation models (SEMs);
- phylosem for comparison among alternative path models;
- phylolm for fitting large linear models that arise as when specifying a SEM with one endogenous variable and multiple exogenous and independent variables;
- Rphylopars for interpolating missing values when specifying a SEM with an unstructured (full rank) covariance among variables;

In model configurations that can be fitted by both phylosem and these other packages, we have confirmed that results are nearly identical or otherwise identified reasons that results differ.

phylosem involves a simple user-interface that specifies the SEM using notation from package sem and the phylogenetic tree using package ape. It allows uers to specify common models for the covariance including:

- Brownian motion (BM);
- Ornstein-Uhlenbeck (OU);
- Pagel's lambda;
- Pagel's kappa;

Output can be coerced to standard formats so that phylosem can use plotting and summary functions form other packages. Available output formats include:

- sem, for plotting the estimated SEM and summarizing direct and indirect effects;
- phylopath, for plotting and model comparison;
- phylo4d in R-package phylobase for plotting estimated traits;

Below, we specifically highlight the syntax, runtime, and output resulting from phylosem and other packages.

Comparison with phylolm

We first compare syntax and run-times using simulated data against phylolm. This confirms that runtimes from phylosem are within an order of magnitude and that results are nearly identical for BM, OU, delta, and kappa models.

```
# Settings
Ntree = 100
sd_x = 0.3
```

```
sd_y = 0.3
b0_x = 1
b0_y = 0
b_xy = 1
# Simulate tree
set.seed(1)
tree = ape::rtree(n=Ntree)
# Simulate data
x = b0_x + sd_x * phylolm::rTrait(n = 1, phy=tree)
ybar = b0_y + b_xy*x
y_normal = ybar + sd_y * phylolm::rTrait(n = 1, phy=tree)
# Construct, re-order, and reduce data
Data = data.frame(x=x,y=y_normal)[]
# Compare using BM model
start_time = Sys.time()
plm_bm = phylolm::phylolm(y ~ 1 + x, data=Data, phy=tree, model="BM" )
Sys.time() - start_time
#> Time difference of 0.001990795 secs
knitr::kable(summary(plm_bm)$coefficients, digits=3)
```

	Estimate	StdErr	t.value	p.value
(Intercept)	-0.371	0.214	-1.734	0.086
X	1.117	0.101	11.053	0.000

Path	VarName	Estimate	StdErr	t.value	p.value
NA	$Intercept_x$	1.087	0.183	5.945	0.000
NA	$Intercept_y$	-0.371	0.213	1.743	0.081
x -> y	p	1.117	0.101	11.109	0.000
x <-> x	V[x]	0.315	0.022	14.072	0.000
y <-> y	V[y]	0.315	0.022	14.072	0.000

```
# Compare using OU
start_time = Sys.time()
plm_ou = phylolm::phylolm(y ~ 1 + x, data=Data, phy=tree, model="OUrandomRoot")
Sys.time() - start_time
```

Path	VarName	Estimate	StdErr	t.value	p.value
NA	Intercept_x	1.028	0.208	4.946	0.000
NA	$Intercept_y$	-0.274	0.235	1.165	0.244
x -> y	p	1.099	0.101	10.887	0.000
x <-> x	V[x]	0.332	0.026	12.712	0.000
y <-> y	V[y]	0.332	0.026	12.860	0.000

knitr::kable(summary(plm_ou)\$coefficients, digits=3)

	Estimate	StdErr	t.value	p.value
(Intercept)	-0.781	0.389	-2.006	0.048
x	1.095	0.101	10.850	0.000

```
\begin{array}{ccc} & & & x \\ \hline phylolm\_alpha & 0.120 \\ phylosem\_alpha & 0.105 \end{array}
```

#> Time difference of 0.08543897 secs knitr::kable(summary(psem_lambda)\$coefficients, digits=3)

Path	VarName	Estimate	StdErr	t.value	p.value
NA	Intercept_x	1.092	0.162	6.740	0.000
NA	$Intercept_y$	-0.346	0.200	1.726	0.084
x -> y	p	1.092	0.103	10.559	0.000
x <-> x	V[x]	0.284	0.025	11.367	0.000
y <-> y	V[y]	0.290	0.024	11.897	0.000

knitr::kable(summary(plm_lambda)\$coefficients, digits=3)

	Estimate	StdErr	t.value	p.value
(Intercept)	-0.356	0.207	-1.718	0.089
X	1.102	0.103	10.744	0.000

	X
phylolm_lambda	0.980
phylosem_lambda	0.957

Path	VarName	Estimate	StdErr	t.value	p.value
NA	$Intercept_x$	1.078	0.186	5.783	0.000
NA	$Intercept_y$	-0.368	0.216	1.705	0.088
x -> y	p	1.113	0.101	11.025	0.000

Path	VarName	Estimate	StdErr	t.value	p.value
x <-> x	V[x]	0.299	0.029	10.183	0.000
y <-> y	V[y]	0.300	0.029	10.343	0.000

knitr::kable(summary(plm_kappa)\$coefficients, digits=3)

	Estimate	StdErr	t.value	p.value
(Intercept)	-0.370	0.216	-1.716	0.089
x	1.115	0.101	11.015	0.000

	x
phylolm_kappa	0.930
phylosem_kappa	0.857

Generalized linear models

We also compare results among software for fitting phylogenetic generalized linear models (PGLM).

Poisson-distributed response

First, we specifically explore a Poisson-distributed PGLM, comparing phylosem against phylolm::phyloglm (which uses Generalized Estimating Equations) and phyr::pglmm_compare (which uses maximum likelihood).

```
# Settings
Ntree = 100
sd_x = 0.3
sd_y = 0.3
b0_x = 1
b0_y = 0
b_xy = 1
# Simulate tree
set.seed(1)
tree = ape::rtree(n=Ntree)
# Simulate data
x = b0_x + sd_x * phylolm::rTrait(n = 1, phy=tree)
ybar = b0_y + b_xy*x
y_normal = ybar + sd_y * phylolm::rTrait(n = 1, phy=tree)
y_pois = rpois( n=Ntree, lambda=exp(y_normal) )
# Construct, re-order, and reduce data
Data = data.frame(x=x,y=y_pois)
```

```
# Compare using phylolm::phyloglm
pglm = phylolm::phyloglm(y ~ 1 + x, data=Data, phy=tree, method="poisson_GEE" )
knitr::kable(summary(pglm)$coefficients, digits=3)
```

	Estimate	StdErr	z.value	p.value
(Intercept)	-1.098	0.633	-1.736	0.083
x	1.314	0.247	5.320	0.000

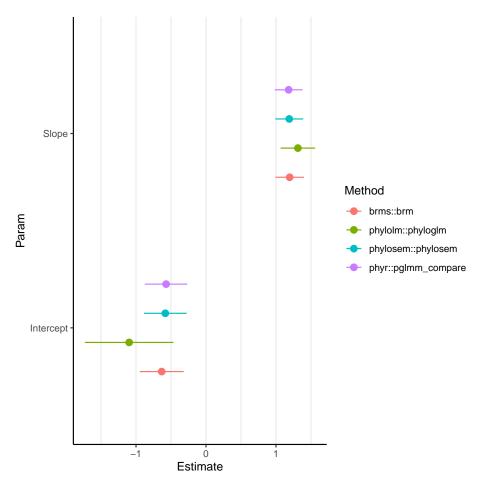
```
pglmm = phyr::pglmm_compare(
 y \sim 1 + x,
 family = "poisson",
 data = Data,
phy = tree )
knitr::kable(summary(pglmm), digits=3)
#> Generalized linear mixed model for poisson data fit by restricted maximum likelihood
#>
\# Call:y \sim 1 + x
#>
#> loqLik AIC BIC
#> -173.4 354.7 360.6
#> Phylogenetic random effects variance (s2):
#> Variance Std.Dev
#> s2 0.05511 0.2348
#> Fixed effects:
               Value Std. Error Zscore Pvalue
#> (Intercept) -0.57009 0.30469 -1.8710 0.06134 .
#> x
             #> ---
#> Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
pgsem = phylosem( sem = "x \rightarrow y, p",
         data = Data,
         family = c("fixed", "poisson"),
         tree = tree,
         quiet = TRUE )
```

Path	VarName	Estimate	StdErr	t.value	p.value
NA	Intercept_x	1.087	0.183	5.945	0.000
NA	$Intercept_y$	-0.581	0.305	1.904	0.057
x -> y	p	1.190	0.199	5.971	0.000
x <-> x	V[x]	0.315	0.022	14.072	0.000
<u>y <-> y</u>	V[y]	0.232	0.054	4.310	0.000

knitr::kable(summary(pgsem)\$coefficients, digits=3)

We also compare results against brms (which fits a Bayesian hierarchical model), although we load results from compiled run of brms to avoid users having to install STAN to run vignettes for phylosem:

```
# Comare using Bayesian implementation in brms
library(brms)
Amat <- ape::vcv.phylo(tree)</pre>
Data$tips <- rownames(Data)</pre>
mcmc <- brm(
  y \sim 1 + x + (1 | gr(tips, cov = A)),
  data = Data, data2 = list(A = Amat),
 family = 'poisson',
  cores = 4
)
knitr::kable(fixef(mcmc), digits = 3)
# Plot them together
library(ggplot2)
pdat <- rbind.data.frame(</pre>
  coef(summary(pglm))[, 1:2],
  data.frame(Estimate = pglmm$B, StdErr = pglmm$B.se),
  setNames(as.data.frame(fixef(mcmc))[1:2], c('Estimate', 'StdErr')),
  setNames(summary(pgsem)$coefficients[2:3, 3:4], c('Estimate', 'StdErr'))
pdat$Param <- rep(c('Intercept', 'Slope'), 4)</pre>
pdat$Method <- rep( c('phylolm::phyloglm', 'phyr::pglmm_compare',</pre>
                      'brms::brm', 'phylosem::phylosem'), each = 2)
figure = ggplot(pdat, aes(
  x = Estimate, xmin = Estimate - StdErr,
  xmax = Estimate + StdErr, y = Param, color = Method
  geom_pointrange(position = position_dodge(width = 0.6)) +
  theme classic() +
  theme(panel.grid.major.x = element_line(), panel.grid.minor.x = element_line())
```



In this instance (and in others we have explored), results from phylolm::phyloglm are generally different while those from phylosem, phyr::pglmm_compare, and brms are close but not quite identical.

Binomial regression

We also compare results for a Bernoulli-distributed response using PGLM. We again compare phylosem against phyr::pglmm_compare, and do not explore threshold models which we expect to give different results due differences in assumptions about how latent variables affect measurements.

```
# Settings
Ntree = 100
sd_x = 0.3
sd_y = 0.3
b0_x = 1
b0_y = 0
b_xy = 1

# Simulate tree
set.seed(1)
tree = ape::rtree(n=Ntree)

# Simulate data
x = b0_x + sd_x * phylolm::rTrait(n = 1, phy=tree)
```

```
ybar = b0_y + b_xy*x
y_normal = ybar + sd_y * phylolm::rTrait(n = 1, phy=tree)
y_binom = rbinom( n=Ntree, size=1, prob=plogis(y_normal) )
# Construct, re-order, and reduce data
Data = data.frame(x=x,y=y_binom)
pglmm = phyr::pglmm_compare(
 y \sim 1 + x,
 family = "binomial",
 data = Data,
 phy = tree )
knitr::kable(summary(pglmm), digits=3)
#> Generalized linear mixed model for binomial data fit by restricted maximum likelihood
#> Call:y ~ 1 + x
          AIC BIC
#> logLik
#> -63.74 135.47 141.32
#>
#> Phylogenetic random effects variance (s2):
#> Variance Std.Dev
#> s2 0.1076 0.328
#>
#> Fixed effects:
#> Value Std.Error Zscore Pvalue
#> (Intercept) 0.23179  0.60507 0.3831 0.7017
#> x 0.44548 0.45708 0.9746 0.3297
```

Path	VarName	Estimate	StdErr	t.value	p.value
NA	Intercept_x	1.087	0.183	5.945	0.000
NA	$Intercept_y$	0.204	0.589	0.346	0.730
x -> y	p	0.458	0.468	0.977	0.328
x <-> x	V[x]	-0.315	0.022	14.072	0.000
y <-> y	V[y]	0.290	0.284	1.020	0.308

In this instance, phylosem and phyr::pglmm_compare give similar estimates and standard errors for the slope term.

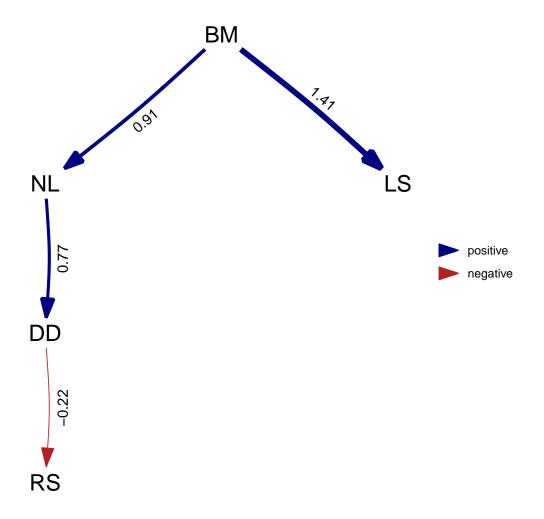
Summary of PGLM results

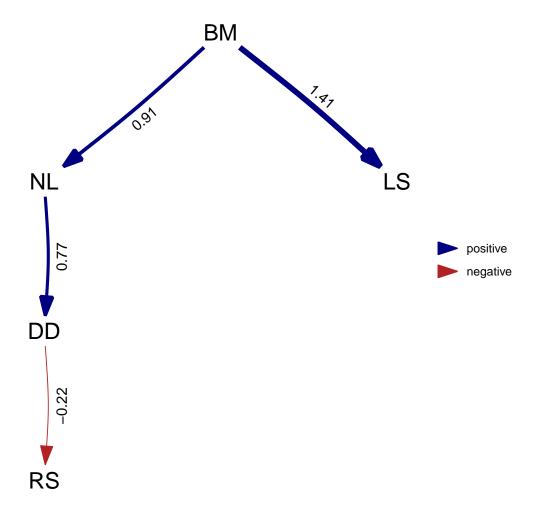
Based on these two comparisons, we conclude that phylosem provides an interface for maximum-likelihood estimate of phylogenetic generalized linear models (PGLM), and extends this class to include mixed data (i.e., a combination of different measurement types), missing data, and non-recursive structural linkages. However, we also encourage further cross-testing of different software for fitting phylogenetic generalized linear models.

Compare with phylopath

We next compare with a single run of phylopath. This again confirms that runtimes are within an order of magnitude and results are identical for standardized or unstandardized coefficients.

```
library(phylopath)
library(phylosem)
# make copy of data that's rescaled
rhino_scaled = rhino
 rhino_scaled[,c("BM","NL","LS","DD","RS")] = scale(rhino_scaled[,c("BM","NL","LS","DD","RS")])
# Fit and plot using phylopath
dag <- DAG(RS ~ DD, LS ~ BM, NL ~ BM, DD ~ NL)
start_time = Sys.time()
result <- est_DAG( DAG = dag,
                    data = rhino,
                    tree = rhino_tree,
                    model = "BM",
                    measurement_error = FALSE )
Sys.time() - start time
#> Time difference of 0.006422997 secs
plot(result)
```





Comparison with sem

We next compare syntax and runtime against R-package sem. This confirms that runtimes are within an order of magnitude when specifying a star-phylogeny in phylosem to match the assumed structure in sem

```
library(sem)
library(TreeTools)

# Simulation parameters
n_obs = 50
# Intercepts
a1 = 1
a2 = 2
a3 = 3
a4 = 4
# Slopes
```

```
b12 = 0.3
b23 = 0
b34 = 0.3
# Standard deviations
s1 = 0.1
s2 = 0.2
s3 = 0.3
s4 = 0.4
# Simulate data
E1 = rnorm(n_obs, sd=s1)
E2 = rnorm(n_obs, sd=s2)
E3 = rnorm(n_obs, sd=s3)
E4 = rnorm(n_obs, sd=s4)
Y1 = a1 + E1
Y2 = a2 + b12*Y1 + E2
Y3 = a3 + b23*Y2 + E3
Y4 = a4 + b34*Y3 + E4
Data = data.frame(Y1=Y1, Y2=Y2, Y3=Y3, Y4=Y4)
# Specify path diagram (in this case, using correct structure)
equations = "
 Y2 = b12 * Y1
 Y4 = b34 * Y3
model <- specifyEquations(text=equations, exog.variances=TRUE)</pre>
# Fit using package:sem
start_time = Sys.time()
Sem <- sem(model, data=Data)</pre>
Sys.time() - start_time
#> Time difference of 0.004453897 secs
# Specify star phylogeny
tree_null = TreeTools::StarTree(n_obs)
  tree_null$edge.length = rep(1,nrow(tree_null$edge))
  rownames(Data) = tree_null$tip.label
# Fit using phylosem
start_time = Sys.time()
psem = phylosem( data = Data,
          sem = equations,
          tree = tree_null,
          quiet = TRUE )
Sys.time() - start_time
#> Time difference of 0.03104401 secs
```

We then compare estimated values for standardized coefficients

	X
b12	0.326
b34	0.325

Path	Parameter	Estimate
Y1 -> Y2	b12	0.345
Y3 -> Y4	b34	0.343

and also compare values for unstandardized coefficients:

	x
b12	0.660
b34	0.390
V[Y1]	0.010
V[Y2]	0.038
V[Y3]	0.098
V[Y4]	0.126

Path	Parameter	Estimate
$\overline{\text{Y1 -> Y2}}$	b12	0.660
Y3 -> Y4	b34	0.390
Y1 <-> Y1	V[Y1]	0.010
Y2 <-> Y2	V[Y2]	0.038
Y3 <-> Y3	V[Y3]	0.098
Y4 <-> Y4	V[Y4]	0.126

Comparison with Rphylopars

Finally, we compare syntax and runtime against R-package Rphylopars. This confirms that we can impute identical estimates using both packages, when specifying a full-rank covariance in phylosem

We note that phylosem also allows parsimonious representations of the trait covariance via the inputted SEM structure.

```
library(Rphylopars)
# Format data, within no values for species t1
Data = rhino[,c("BM","NL","DD","RS","LS")]
  rownames(Data) = tree$tip.label
Data['t1',] = NA
# fit using phylopars
start_time = Sys.time()
pars <- phylopars( trait_data = cbind(species=rownames(Data),Data),</pre>
                  tree = tree,
                  pheno_error = FALSE,
                  phylo_correlated = TRUE,
                  pheno_correlated = FALSE)
Sys.time() - start_time
#> Time difference of 0.0739851 secs
# Display estimates for missing values
knitr::kable(cbind( "Estimate"=pars$anc_recon["t1",], "Var"=pars$anc_var["t1",] ), digits=3)
```

	Estimate	Var
$\overline{\mathrm{BM}}$	1.266	1.941
NL	1.600	1.856
DD	2.301	1.708
RS	0.431	1.909
LS	1.083	1.347

Estimate	Var
1.266	1.941
1.600	1.856
2.301	1.708
0.431	1.910
1.083	1.347